2,2,3,3,4,4,5,5,6,7,7,7-Dodecafluoro-6-(trifluoromethyl)heptanoic acid

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 8.54e-01 mol/L

Global applicability domain: Outside

Local applicability domain index: 2.11e-01

Confidence level: 4.98e-01

Nearest Neighbors from the Training Set

Image not found

Fluopropanate-sodium
Measured: 1.31e-01
Predicted: 4.65e-01

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Acetic acid, trifluoro-
Measured: 8.77
Predicted: 4.36

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1,1,1-Trifluoro-2-propanol
Measured: 2.04
Predicted: 2.45

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2,2,2-Trifluoroethanol
Measured: 10.0
Predicted: 6.34